FINITE ELEMENT MODELING OF STRESS-INDUCED β→ω TRANSFORMATION IN β TITANIUM

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Abstract

Titanium alloys are materials exhibiting outstanding physical and functional properties. Metastable β titanium alloys are a prospective group featuring complex phase transformations which can be utilized to tailor the material performance. Microstructural mechanisms underlying phase transformations in this group of Ti alloys are not completely understood. In particular, the formation of different morphologies of ω phases is of major importance as the ω particles act as nucleation sites for the formation of stable α phase. In this study, we employ a finite element model (FEM) to account for the formation of two types of ω phase, namely, the ellipsoidal athermal ω phase and the lamellar stress-induced ω phase. The proposed model calculates elastic strain energies in β titanium containing either athermal or stress-induced ω phase and, thus, determines the preferential morphology of the formed ω phase in relation to the stress magnitude and direction.

Keywords: β titanium, ω phase, FEM, phase transformation

1. INTRODUCTION

Titanium and its alloys, owing to their exceptional mechanical performance (e.g. specific strength and fatigue resistance), corrosion resistance and biocompatibility [1], have been recently attracting substantial scientific interest. There has also been an increased demand for these materials in the medicine, aerospace, automotive and chemical industries. Titanium is an allotropic metal which undergoes a phase transformation at 882°C from the low temperature α phase (hcp) to the high temperature β phase (bcc). This temperature can be influenced by additions of alloying elements and the resulting alloys and their phase composition at room temperature can be divided into four categories, namely α, α+β, metastable β and stable β alloys. Metastable β titanium alloys have attracted the attention of researchers as their microstructure and mechanical properties can be effectively tailored by thermo-mechanical treatment [2-5]. In these alloys, the bcc β phase is retained in a metastable state during quenching and further undergoes several complex phase transformations which involve different mechanisms [6]. Metastable ellipsoidal particles of athermal omega (ω_{ath}) phase are commonly formed in less-stabilized metastable β alloys during quenching [7,8]. ω_{ath} particles are finely distributed and their size is typically 1-2 nm [9,10]. Another type of phase in metastable β alloys is the stress-induced lamellar ω phase [11, 12]. Moreover, alpha precipitation (α_{nano}) can occur at elevated temperatures exploiting the ω particles as nucleation sites. These transformations open new possibilities of controlling the microstructure through optimized heat treatments and mechanical preloading. However, understanding of mechanisms underlying the evolution of these phases is rather incomplete.

Finite element modeling (FEM) method is proposed in this work to evaluate conditions for the formation of stress-induced and athermal ω phases in metastable β titanium, i.e. to consider the effect of ω phase morphology on the resulting microstructure. Based on the calculations of elastic strain energies in the alloy

containing ω phase ellipsoids (athermal ω) or ω phase lamellae (stress-induced ω), the preferential formation of these phases can be assessed.

2. β→ω PHASE TRANSFORMATION AND FEM MODEL

Athermal and stress-induced β→ω phase transformations were investigated by numerical simulation using the FEM method. FEM is a well-established and commonly used technique for solving boundary condition problems in many fields of materials science. It is also a suitable tool to obtain elastic strain energies after diffusionless phase transformations in metals. The model proposed in this study was implemented in the Comsol Multiphysics and Matlab software packages.

The β titanium phase crystallizes in a body-centered cubic (bcc) structure while the ω phase has a hexagonal (hex) structure. The displacive β→ω phase transformation can be formally described as two neighboring $(111)_\beta$ planes collapsing into their intermediate position while the adjacent $(111)_\beta$ planes remain unchanged. Another two following planes collapse again and so on (see **Figure 1**) [13, 14]. Owing to the symmetry of this transformation, a specific orientation relationship exists between the new ω lattice and the parent β phase. The lattice parameters of the newly formed ω phase can be geometrically expressed as [13, 14]:

$$a_\omega = \sqrt{2}\, a_\beta; \quad c_\omega = \sqrt{3}/2\, a_\beta \tag{1}$$

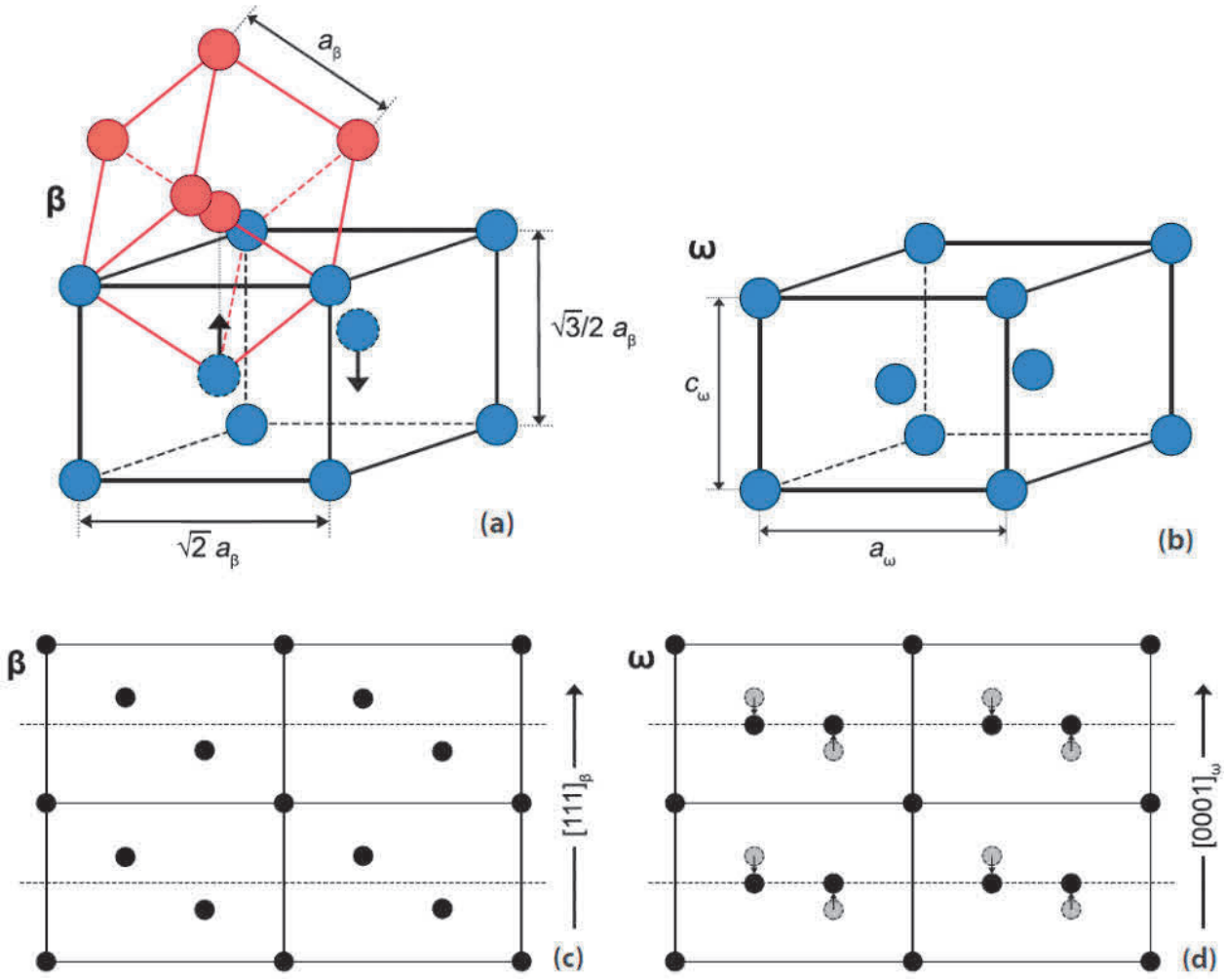

Figure 1 3D schematic view of displacive β→ω phase transformation: (a) β phase and (b) transformed ω phase; and 2D view of (c) β phase and (d) transformed ω phase [13]

The geometrically expressed ω phase lattice parameters deduced from the β phase do not perfectly match the experimental values. This occurs due to the lattice distortion as a result of atomic shift during phase transformation. In the FEM model, this effect can be accounted for by using non-zero initial strains in the ω phase, which were calculated to be ε_{xx} = -0.0109 and $\varepsilon_{yy} = \varepsilon_{zz}$ = 0.0046. Lattice parameters of the β phase (a_β = 0.328 nm) and the athermal ω phase (a_ω = 0.467 nm, c_ω = 0.281 nm) were obtained from the literature [15]. Main directions in the model coincide with the lattice axes of the ω phase (c_ω || x and a_ω || y). It should be mentioned that FEM model used in this work does not account for plastic deformation. For the sake of simplicity, the proposed model considers only one crystallographic variant of the ω phase, while four equivalent variants exists due the symmetry of bcc β phase.

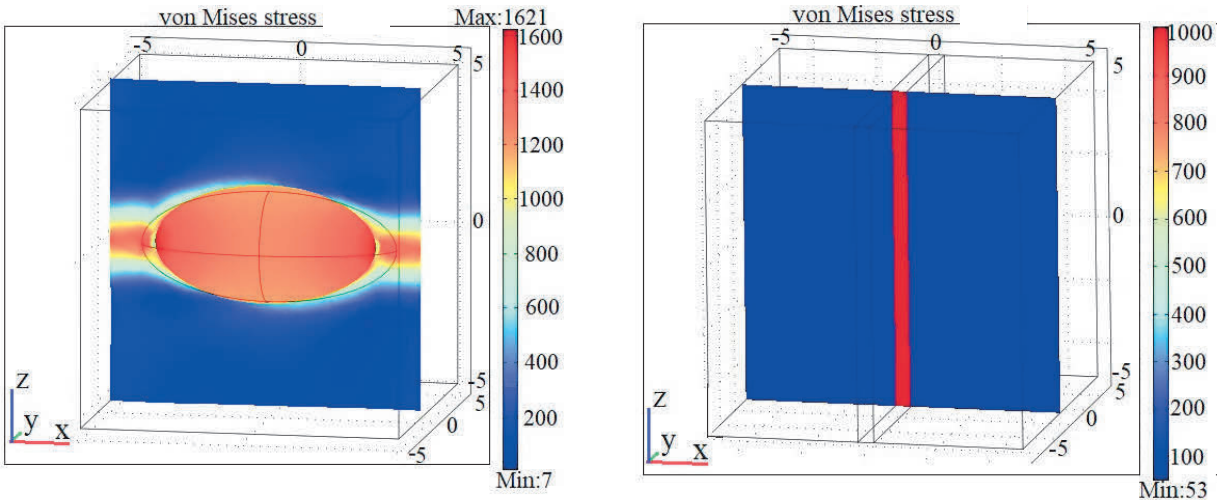

Figure 2 Cross section of the modelled area showing the von Mises stresses in β titanium containing (left) athermal ellipsoidal ω phase and (right) stress-induced lamellar ω phase

In order to obtain elastic strain fields, the knowledge of elastic constants, C_{ijkl}, of both phases is required. The constants used in the model were taken from the literature [16,17]. Two model geometries were implemented. In the first model, ellipsoidal athermal ω phase (as observed experimentally in quenched β titanium [18,19]) was considered while the second one assumed ω lamellae, which represent the stress-induced ω phase [20,21]. The modelled region had the dimensions of 10×10×10 nm^3 (**Figure 2**) and 5 vol.% of the β phase underwent the β→ω phase transformation in both cases. The length of principal axes of the ellipsoid (prolate spheroid) was a = b = 3.455 nm and c = 8 nm; and the width of the lamella was 0.5 nm. Periodic boundary conditions were used for all directions of the modelled region. This criterion ensures the particles are periodically arranged in an infinite β phase.

3. MODEL RESULTS AND DISCUSSION

According to the simulation results, the direction of applied load significantly affects the strain energies in both cases, i.e. in the presence of the ω phase ellipsoidal particles and the ω phase lamellae (**Figure 3**). The red hexagon-based prism represents the lattice of the ω phase and the blue cube represents properly oriented β lattice with respect to the ω phase. Significant variation in the elastic energies can be explained by the anisotropic properties of the two phases and their relative misorientation. **Figure 3** shows the elastic energy as a function of applied stress in 3 different directions, $[100]_\beta$, $[11\text{-}20]_\omega$ and $[0001]_\omega$. The schematic illustrations on both sides of **Figure 3** demonstrate the directions of the applied stress for each curve representing lamellar (red curves, left side illustrations) and ellipsoidal (black curve, right side illustrations) ω phase. The transparent red lamellae (left) and ellipsoids (right) indicate the ω phase orientation. At zero external stress, the elastic strain energy is slightly lower in β titanium with ω lamellae ($\Delta E_{e0} = E_{ellips} - E_{lam}$ = 0.84 eV). On the other hand, it

was shown experimentally that lamella-shaped ω phase can be formed only under external load [20, 21]. In order to find correlations between calculated elastic energies and preferential formation of different types of ω phase, the total energy, i.e. the sum of elastic and surface energy (E=E_e+E_s), need to be considered. The surface energy E_s between the two phases, β and ω, is proportional to the interface surface, S: E_s = S·e_s, where e_s is the surface energy density.

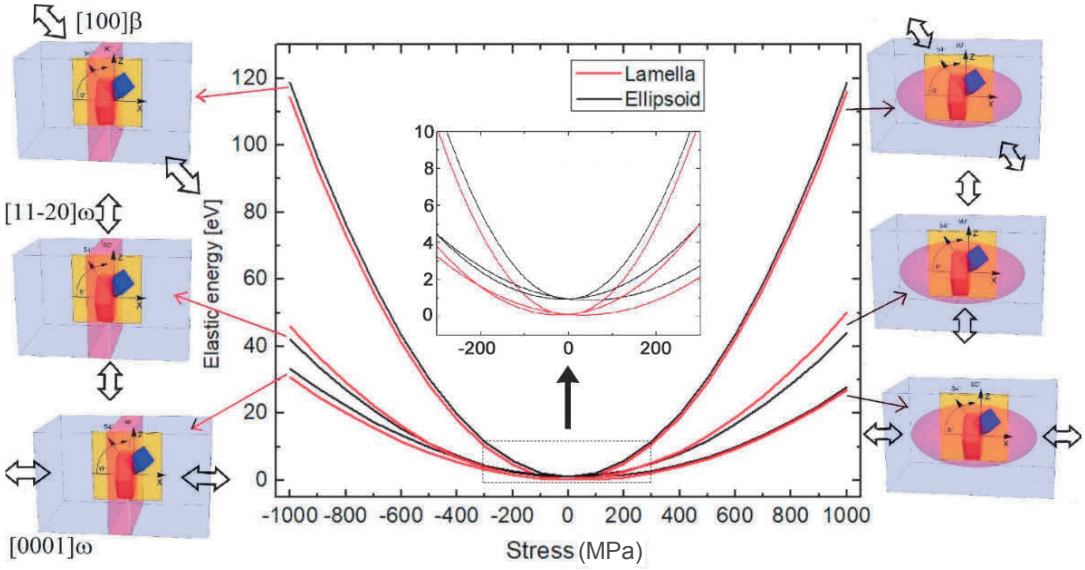

Figure 3 Elastic deformation energy in the β phase containing ellipsoidal (black) and lamella-shaped (red) ω phase as a function of applied stress in three different directions. Side illustrations show the orientation of phases and the direction of applied load

The interface surface area of lamellar ω phase (S_{lam}) is larger than the surface area of ellipsoidal ω particle (S_{el}). The surface area difference is ΔS = S_{lam}-S_{el} = 200-72.87 = ~127 nm^2, resulting in increased total elastic energy in the laminate. Studies of surface energy at the β/ω interface are missing in the literature. However, some experimental and theoretical results concerning the average surface energy [22] and the stacking fault energies [22, 23] of titanium were reported. It is assumed that the stacking fault energy density, e_{SFE}, which varies between 24-300 mJ/m^2 (~0.15-1.87 eV/nm^2), is of the same order as the β/ω interface energy density. According to this assumption, the difference in the surface energies of ω particles found is this study will be ΔE_s = ΔS·e_{SFE} = ~19-240 eV. Therefore, the formation of ω lamellae can be favored in a wide range of external stress values when surface energies are taken into account. As the elastic energy difference in the initial unloaded state (ΔE_{e0} = ~1 eV) is lower than the lowest possible value of ΔE_s, the ellipsoidal phase particles will be energetically more advantageous. Due to the absence of surface energy studies of the ω phase in the literature, the exact stress levels at which the lamellae will form instead of the ellipsoidal particles cannot be assessed. On the other hand, if the elastic strain energy difference between the two modifications of the ω phase, ΔE_e, is investigated (see **Figure 4**), the conditions, at which either lamellar or ellipsoidal omega particles are more likely to form, may be estimated.

The difference in the elastic energies, ΔE_e=E_{ellips}-E_{lam}, changes with varying external load. The larger the value of ΔE, the higher the chance of formation of lamellae instead of ellipsoidal particles. In **Figures 4a-c**, the applied load in three different planes, XZ, YZ and XZ (marked in yellow) was simulated at different angles φ with respect to one of the axes. Due to the common mirror symmetries around the examined angle, the φ ranges were 0-90° (XY plane) or 0-180° (YZ and XZ planes).

The load direction in the XY and XZ planes has a significant effect on the evolution of ΔE_e. It was found out that the angle around φ_{xz} = 70° (i.e. the direction between $[100]_\beta$ and $[11\text{-}20]_\omega$) in the XZ plane (**Figures 4c**

and **d**) might be the most favorable for the formation of lamellar structure among all simulated directions. By changing the load direction from 70° in the XZ plane, ΔE_e rapidly decreases and reaches a minimum around 135°, which suggests that the formation of ω lamellae might be suppressed. In the XY plane (**Figure 4a**), the ΔE as a function of loading direction exhibits monotonic behavior. The largest positive ΔE_e values are obtained in the direction of $\varphi_{xy} = 0°$ ($[10\text{-}10]_\omega$ or $[110]_\beta$), then the difference of surface energies gradually decreases and the smallest value is observed for $\varphi_{xy} = 90°$, i.e. in the $[0001]_\omega$ direction. In the YZ plane (**Figure 4b**), which is equivalent to the basal plane of the ω phase, no such a strong difference was observed in different load directions as all ΔE curves were similar. This is most likely caused by a constant initial strain ($\varepsilon_{yy} = \varepsilon_{zz}$) in this plane. The obtained results suggest that the most favorable orientation for the formation of lamellar ω phase is when the crystal is loaded along the basal plane of the ω phase. Another interesting result is that in compression slightly higher ΔE values are evidenced at the same applied compression/tension load levels. Therefore, there is a higher chance for the formation of lamellae for all investigated load directions in compression when compared with simulation results in tension.

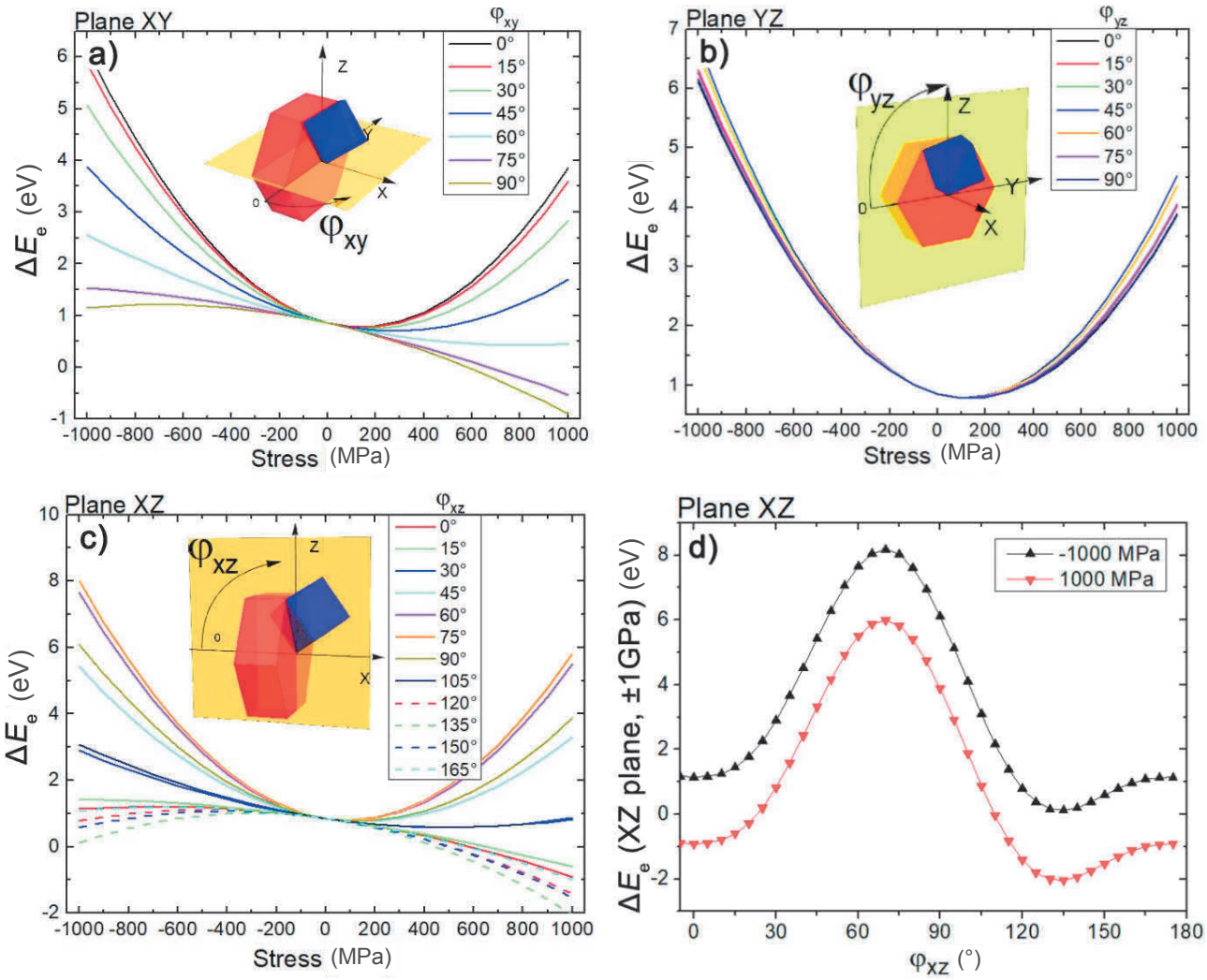

Figure 4 Difference in the elastic energy, $\Delta E_e = E_{ellips}\text{-}E_{lam}$, as a function of external load in the direction from a) y to x axis b) x to z axis and c) y to z axis. Graph d) shows ΔE_e under uniaxial compression and tension in different directions, φ_{xz}

More accurate predictions of preferential formation of the ω phase ellipsoids or lamellae would be possible if more precise values of surface energies were estimated. Inclusion of surface energies and comparison of the results with experimental data are challenges for the future work.

4. CONCLUSIONS

In this work, the β→ω transformation was investigated in β titanium by FEM numerical modeling. The aim of the study was to find relations between the evolution of elastic strain energies of lamellar (stress-induced) and ellipsoidal (athermal) ω particles and the conditions for their formation. The following main conclusions can be drawn:

- Calculated elastic strain energies in β titanium can help to predict preferential formation of the ω phase in the form of lamellae or ellipsoidal particles.
- According to the model results, the direction of applied external load is an important factor in the prediction of which modification of the ω phase is more likely to form. The most favorable orientation for the formation of ω lamellae is when the load is applied along the basal plane of the ω phase.
- The calculation of elastic strain energies is not sufficient to predict exact stress values at which the preferential formation of either ω phase modification will occur. For this purpose, surface energies have to be also taken into account.

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